LA-UR-15-27387
Approved for public release; distribution is unlimited.

Title: Evaluation of PRZ in FLAG

Author(s): Quirk, James J.
Meyer, Chad D.

Intended for: PEM/HE L2 Milestone

Issued: 2015-09-22

Evaluation of PRZ in FLAG

PEM/HE L2-Milestone 2015

James Quirk & Chad Meyer

XCP-4 Methods & Algorithms
Los Alamos National Laboratory
Los Alamos, NM 87545

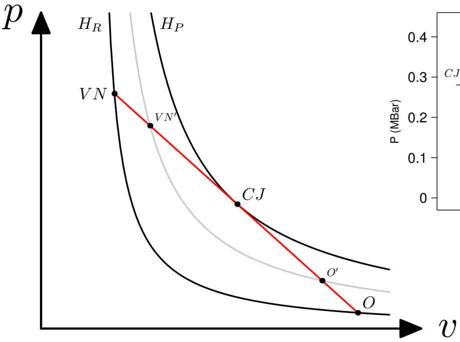
September 24, 2015

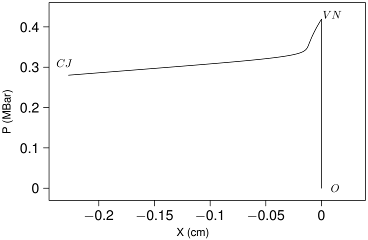
Outline

- Verification: is FLAG's PRZ implemented correctly?
  - Examine piston-driven ZND wave
    - introduce some practical considerations
    - introduce length scales
    - check P-T and P-RHO closures
    - check mesh convergence
- Evaluation: how well does FLAG's PRZ perform?
  - Revisit piston-driven ZND wave
    - show canonical errors of programmed burn
    - show sensitivity to initial conditions
  - Examine cylindrical detonation
    - show consequences of PRZ formulation
  - Examine slab, ratestick, and arcwave detonations
    - show interplay between PRZ and FLAG-hydro
- Summary: what have we learnt?

Is FLAG's PRZ implemented correctly?

- Check PRZ[7] detonation, for Davis wide-ranging EOS[8], against Zel'dovich – von Neumann – Döring steady, travelling-wave solution[4]
  - The minimum-entropy solution: an inert shock compresses state *O* to state *VN* then reaction proceeds to sonic-state *CJ*





  - As with any programmed-burn method, there are complications which will be addressed later on

FLAG: some practical considerations

- There are six different ways to account for the detonation energy
  - moreover they are not all equivalent with one another

```
mk /global/mesh/mat(mat1)/gas/element/hepoly
   heenergy = @heenergy

mk /global/mesh/mat(mat1)/gas/model/twoeoss
   e0_1 = @e0_1  $ broken in parallel
   e0_2 = @e0_2  $ broken in parallel

mk /global/mesh/mat(mat1)/gas/model/twoeoss/eos1
   e0 = @e0_1
mk /global/mesh/mat(mat1)/gas/model/twoeoss/eos2
   e0 = @e0_2    $ preferred way
mk /global/mesh/mat(mat1)/gas/model/twoeoss/eos2/davisprod
   ener0 = @ener0
```

- Employ test harness to run through energy variations
  - Allows parameter studies via a templated FLAG input-deck
  - Fully automated to allow studies to be redone when required

FLAG: some practical considerations (contd.)

- PRZ is a programmed-burn methodology, it requires:
  - A burn-table, tb, to dictate when the reaction starts
  - A detonation-velocity-table, Dn, to dictate the reaction scaling

    $rate1,2 \propto \left(\frac{Dn}{D_{CJ}}\right)^{n1,n2}$; two rates to allow for fast/slow reactions
- The tb and Dn tables are computed independently of FLAG
  - The 1D tests here use analytic tables:

$$Dn = D_{CJ}; \qquad tb = \frac{x}{Dn}$$

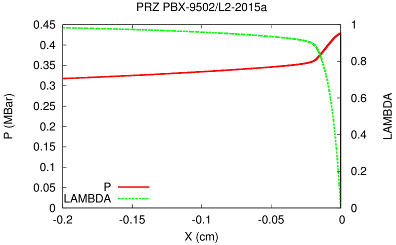
  - The 2D tests use tables computed via a body-fitted, DSD code
  - The tables are read into FLAG using:

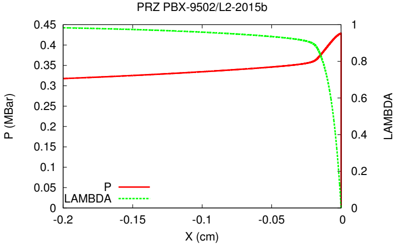
```
/global/mesh/heburn/heread_btdv
   file = @burntable
```

- The test harness employs two passes
  - Pass one: invoke FLAG to setup test-problem and dump geometry
  - Pass two: prepare tables and run FLAG on test-problem

PRZ: length scales

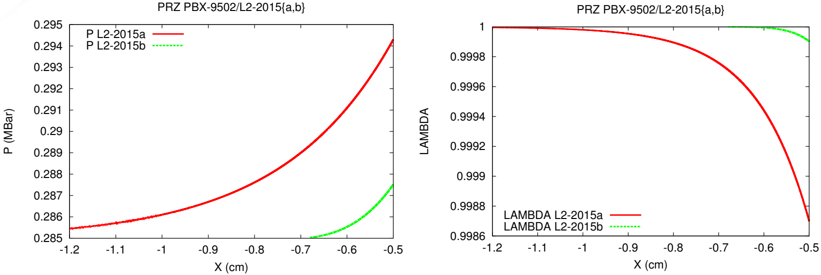
- ZND solutions can be obtained semi-analytically
  - Reduce problem to an ODE in λ and integrate $\lambda : 0 \rightarrow 1$
- PRZ mimics the length scales in a full reactive burn model
  - For PBX-9502: 38μm half-reaction; $\approx$ 2000μm burnout
  - Two calibrations for L2-milestone[2, 1]
    - one with a finite-reaction length, one without
    - differences near CJ point are not seen here





PRZ: length scales (contd.)

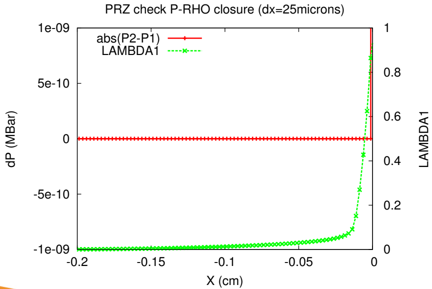
- Difference in PRZ calibrations visible near CJ point
  - Linear burnout for calibration L2-2015a[2] motivated by chemistry, but results in infinitely long reaction length

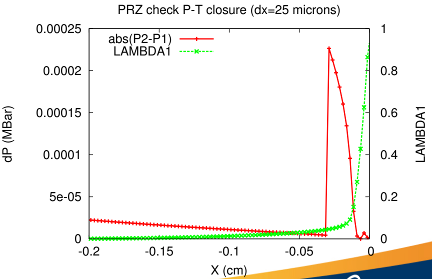


    - implications for various thresholds and tolerances used by FLAG
- A detonation is a coupled hydrodynamic-reactive system
  - Numerical cut-offs at the CJ state affect wave speed

FLAG: check P-T/P-RHO closures

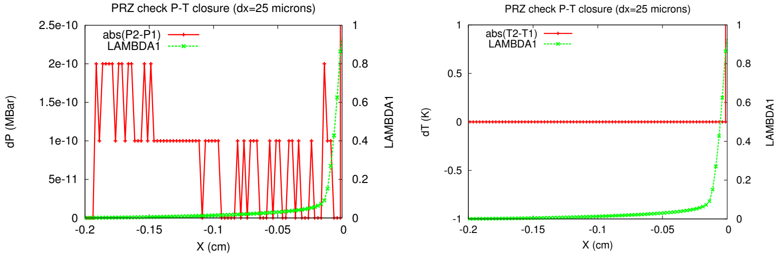
- As with a reactive burn model, PRZ requires a closure to partition energy between reactants and products
  - FLAG currently allows for both P-T and P-RHO closures
    - the L2 calibrations employed P-T equilibrium as P-RHO was not available in FLAG at the time they were done
- To verify FLAG: prescribe ZND solution and march one step
  - P-RHO closure is correct to 10 significant figures, but hard-wired tolerances in P-T solver are too coarse





FLAG: check P-T/P-RHO closures (contd.)

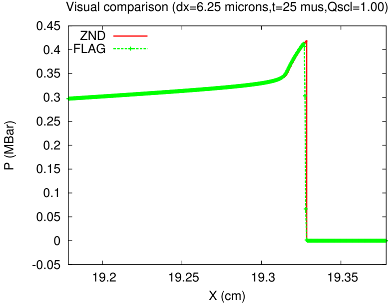
- The P-T closure is computationally more involved than P-RHO
  - It involves a nested solve that can fail to converge
- Tightening FLAG's tolerances allows this test to be passed
  - Compiled custom code with: abs_error=1e-9, rel_error=1e-12

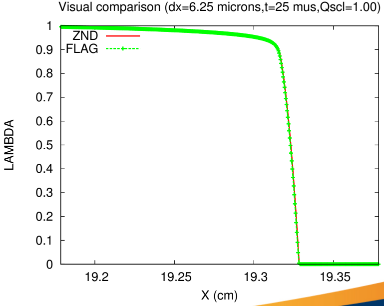


- Observe sporadic warnings that P-T solve has not converged
  - Further investigation needed

ZND: check mesh convergence

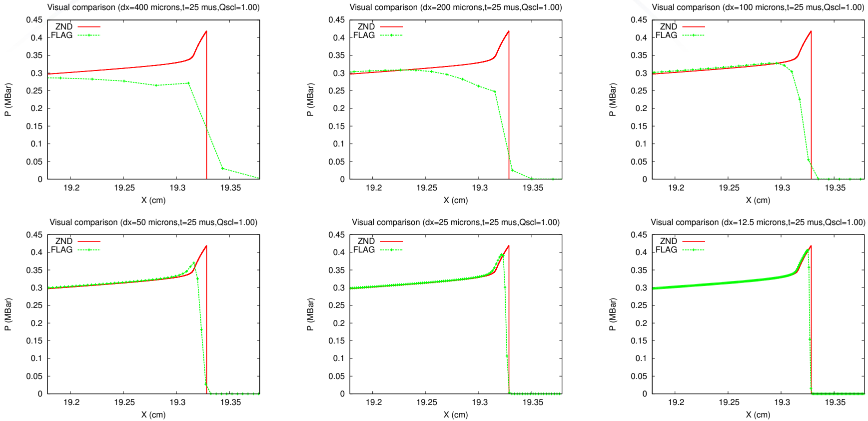
- A mesh convergence study, repeatedly halving dx from 400μm to 6.25μm, shows PRZ is implemented correctly
  - done for three PBX-9502 calibrations[2, 1, 8]
  - done for both P-T and P-RHO closures
  - done for four of FLAG's six energy input-variations
  - 168 cases in total (7 x 3 x 2 x 4)
- Visual check for $dx = 6.25\mu m$, calibration[1], P-T closure, and e0_2





ZND: check mesh convergence (contd.)

- Programmed-burn is intended to be run on coarse meshes[6]
  - outside of the asymptotic range of the PRZ model



ZND: check mesh convergence (contd.)

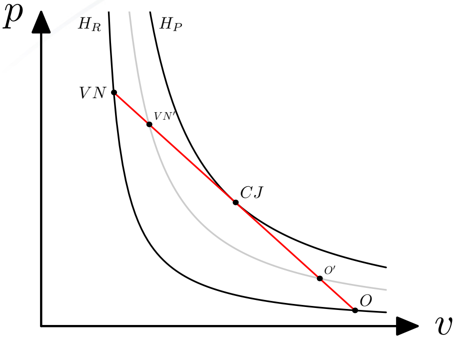
- Formal error norms are not presented here
  - They are misleading in the context of programmed-burn
    - for $dx > 50\mu m$ the details of the calibration are lost
  - Computational errors vary with the run length of the detonation
    - synchronization errors are slowly evolving and can be missed when the run length is too short
    - would need to present norms at $1, 10, 100, \ldots \mu s$
  - Local errors tend to dominate the norm
    - a numerical cut-off at the CJ point can be troublesome
  - Errors are often *glaring*
    - *footing* when the burn-table is too fast
    - *flat-top* when the burn-table is too slow
  - FLAG's evolution of λ is known to be weak
    - two forward-Euler integrations, with a half-time step, are used
    - should migrate to predictor-corrector or two-stage Runge-Kutta

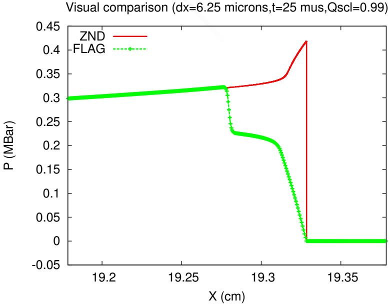
How well does FLAG's PRZ perform?

- As with any programmed-burn method, PRZ does not model the coupling found in a real detonation
  - Synchronization of the reaction with the hydro is always an issue
    - no mechanism to maintain synchronization
    - need to check what happens when the burn table is too fast
    - need to check what happens when the burn table is too slow
  - The initial conditions used to start a simulation are problematic
    - no mechanism to grow a detonation from nothing
    - therefore must prescribe an initial detonation profile
    - or play tricks with the burn table to obtain a lead shock
- PRZ is only as good as its burn table, which in turn is only as good as the Dn-Kappa calibration
  - EOS parameters, PRZ parameters, and Dn-Kappa parameters have to be consistent
    - users are not free to *pick-and-mix*

Canonical-error: burn table is too fast

- When the burn table is too fast:
  - Shock-less burning will appear ahead of the detonation i.e. *footing*

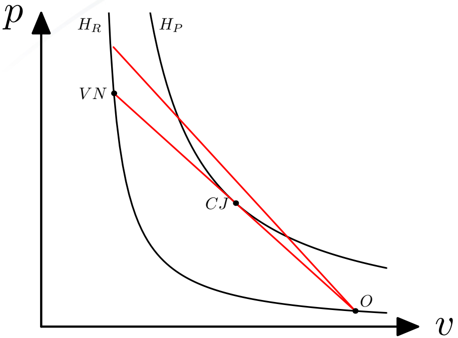


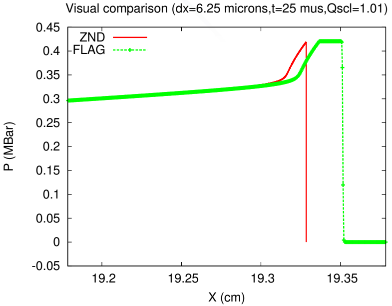


  - Wilkins's traditional programmed-burn is by design *shock-less*[6]
    - this is achieved via the EOS modification $e = e(\rho, P/\lambda, \lambda)$
    - but on coarse grids computations *appear* to involve a shock

Canonical-error: burn table is too slow

- When the burn table is too slow:
  - A shock runs ahead of the reaction region, resulting in a *flat-top*

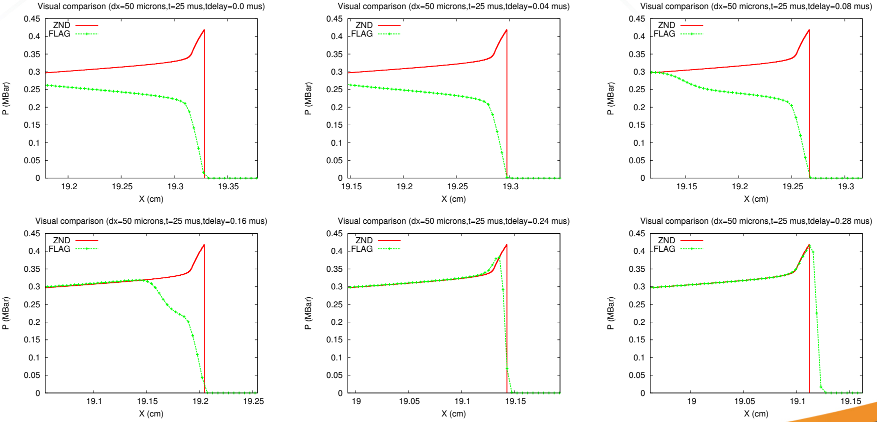




  - An argument can be made for biasing a PRZ burn-table to be on the slow side, so as to avoid *footing*
    - but is the cure worse than the disease?

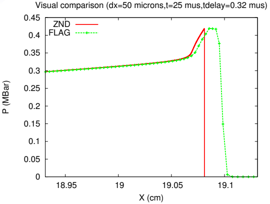
Initial conditions are problematic

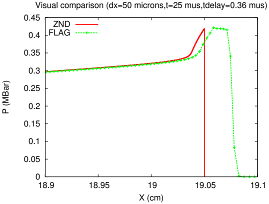
- The ZND test can be repeated using just quiescent initial conditions, with a delay in the burn-table
  - Shock-less burning is observed when the delay is less than $0.28\mu s$

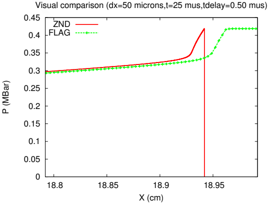


Initial conditions are problematic (contd.)

- The ZND test can be repeated using just quiescent initial conditions, with a delay in the burn-table
  - A *flat-top* is observed when the delay is greater than $0.28\mu s$







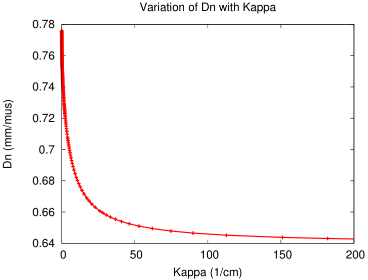
- Biasing a burn table to be too slow provides a simple means of avoiding shock-less burning
  - Requiring users to initialise with a ZND profile is likely a non-starter
  - A delay of $0.28\mu s$ corresponds to $2.18mm$
  - The delay for a CJ-blob as initial conditions is $0.1\mu s$

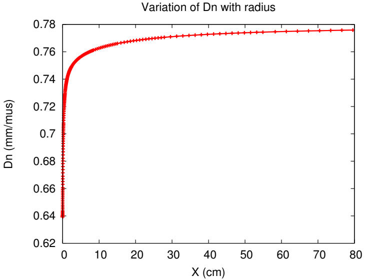
Cylindrical detonation

- The motivation for DSD[3, 5] is that curved detonations propagate at appreciably slower speeds than the CJ velocity dictated by 1D theory†
  - The assumed formulation for $Dn(\kappa)$ is:

$$\frac{D_n}{D_{CJ}} = 1 + A\left[(C_1 - \kappa)^{E_1} - C_1^{E_1}\right] - B\kappa\frac{(1 + C_2\kappa^{E_2} + C_3\kappa^{E_3})}{(1 + C_4\kappa^{E_4} + C_5\kappa^{E_5})}$$

  - The calibration for PBX-9502[5] can be integrated to get tb and Dn tables so as to test PRZ on a cylindrically expanding detonation

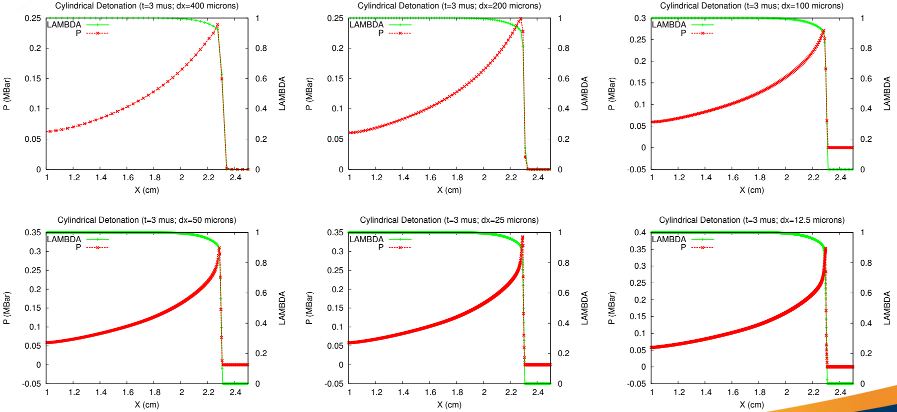




† The DSD theory is strictly only valid for positive curvature

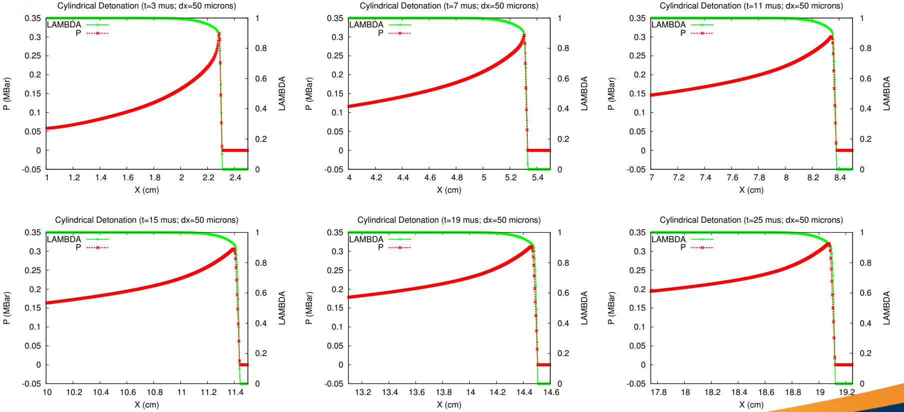
Cylindrical detonation: early time convergence

- A mesh convegence study, repeatedly halving dx from 400μm to 12.5μm, shows PRZ is prone to give shockless burning
  - The *footing* is most prounounced in the lower-right plot
    - all the results here are for $t = 3\mu s$



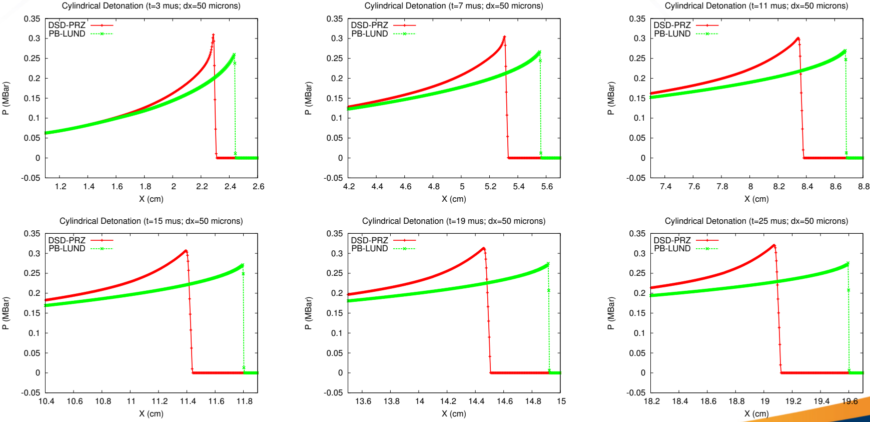
Cylindrical detonation: evolution

- The numerical evidence is that even when a shock is present at early-time, PRZ will gravitate to shockless burning at late-time
  - The amount of shock-less burning increases with time
    - all the results here are for $dx = 50\mu m$



Cylindrical detonation: PRZ vs. PB

- PB, with LUND, propagates a cylindrical detonation at constant speed, which is physically unrealistic and overpredicts the front position
  - But unlike DSD-PRZ, LUND-PB is not prone to shockless burning
    - what is happening with PRZ?

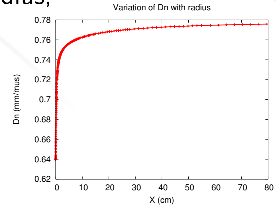


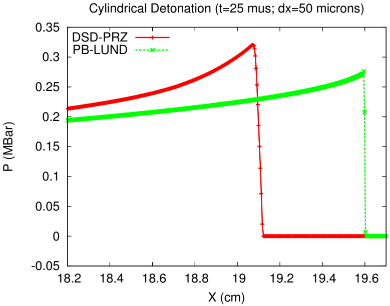
Cylindrical detonation: a PRZ weakness

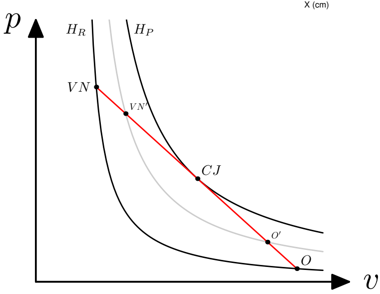
- PRZ has the wrong functional form to maintain the lead shock
  - From the Dn-Kappa curve, Dn increases with radius,

    but PRZ has $rate1,2 \propto \left(\frac{Dn}{D_{CJ}}\right)^{n1,n2}$

    - a particle engulfed at radius, r, burns more slowly than one engulfed at, $r + dr$, and so shockless burning is inevitable

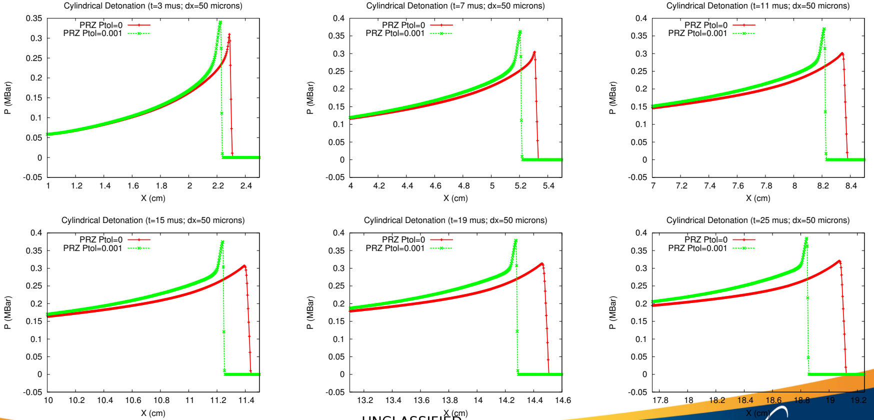






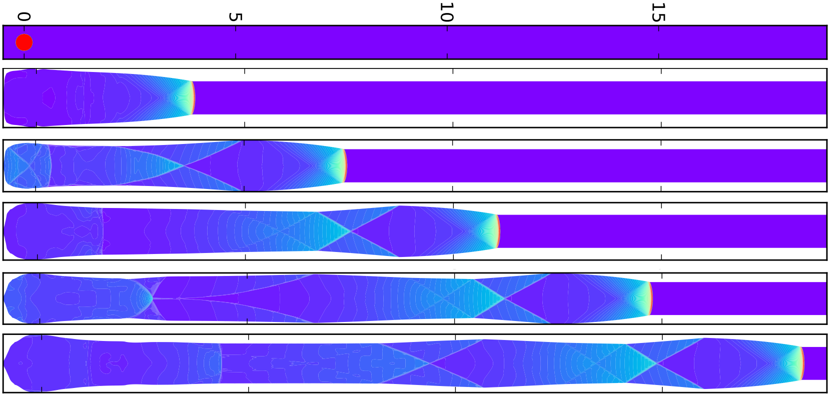
Cylindrical detonation: how to fix PRZ?

- For reactive-burn models it is common to employ a pressure threshold to prevent burning in the numerically-smeared, lead shock
  - This approach prevents PRZ from giving shockless burning
    - at the cost of circumventing the tb table i.e. lighting is dictated by the hydro with the reaction-rate scaled via the Dn table



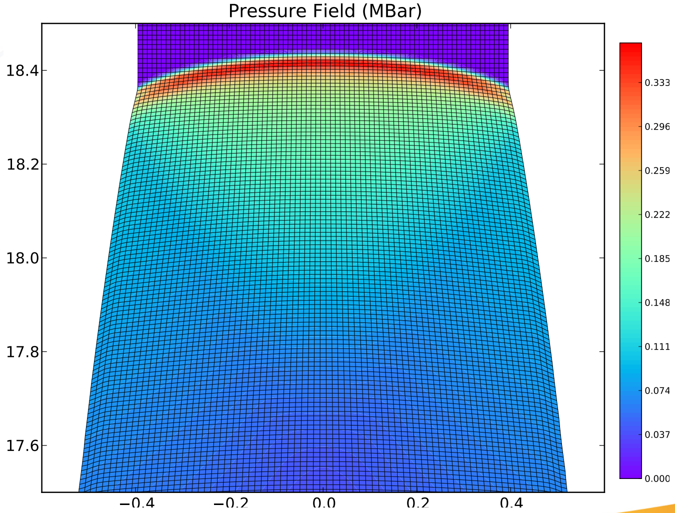
Slab detonation

- DSD-PRZ simulations have been performed in FLAG for an 8mm slab of PBX-9502[5], with the three available calibrations[8, 2, 1]
  - Pressure results for calibration[1] with $dx = 50\mu m$
    - reflected shocks arise because FLAG does not have an outflow-BC



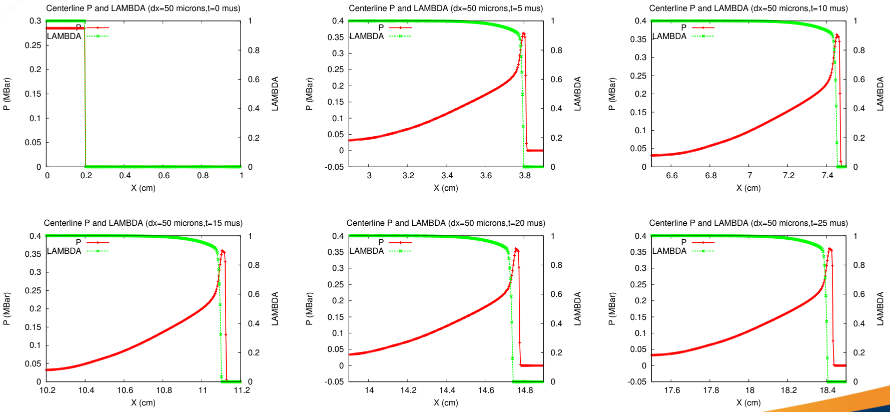
Slab detonation: zoom of the front

- Qualitatively the results are the same for all three calibrations
  - Unlike Lund programmed-burn, the detonation front is curved



Slab detonation: evolution along centreline

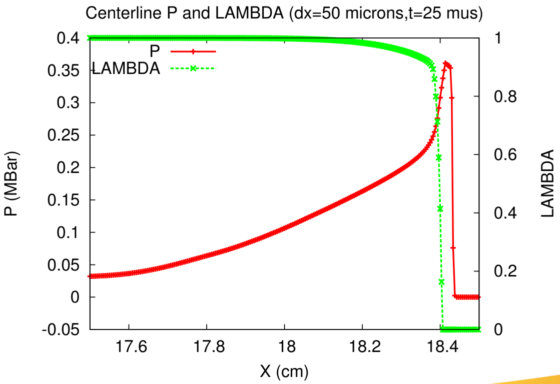
- The burn-table employs a Dn-Kappa curve calibrated to experiment[5]
  - The *validation* of the DSD-PRZ methodology hinges on whether the FLAG hydro can remain synched with the burn-table
    - results at $dx = 50\mu m$ indicate a *flat-top* error



UNCLASSIFIED

Slab detonation: proportioning of errors

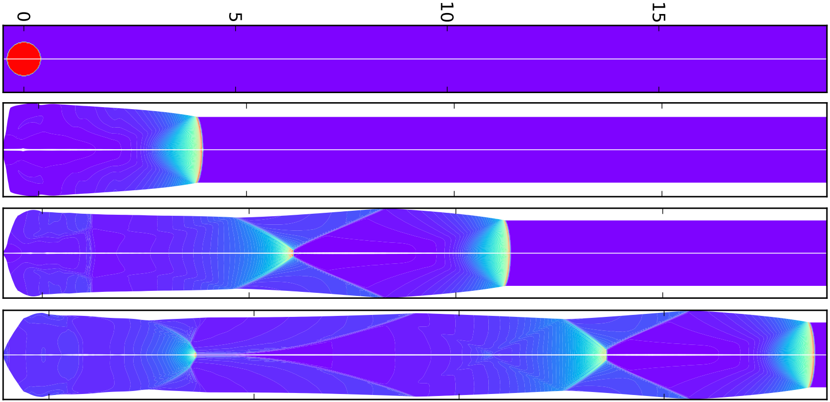
- Further investigation is needed to proportion the error
  - DSD vs. PRZ vs. FLAG vs. mesh resoluton vs. ...
  - Compared to the cylindrical case shockless burning is inhibited because Dn reaches steady state
    - but it could reappear for fine mesh simulations



UNCLASSIFIED

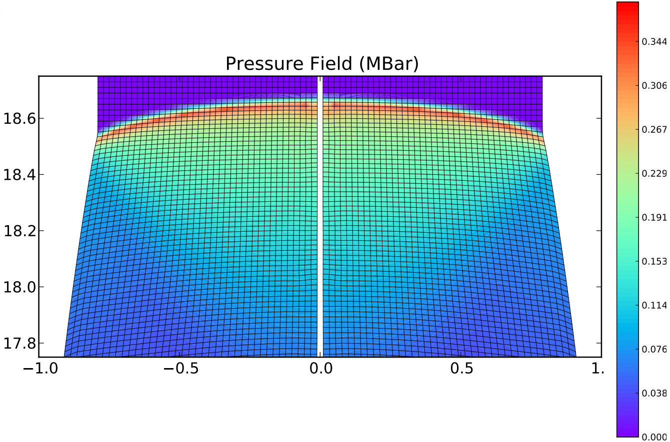
Ratestick detonation

- DSD-PRZ simulations have been performed in FLAG for a 16mm diameter ratestick of PBX-9502, with the three calibrations[8, 2, 1]
  - Pressure results for calibration[1] with $dx = 100\mu m$
    - reflected shocks arise because FLAG does not have an outflow-BC



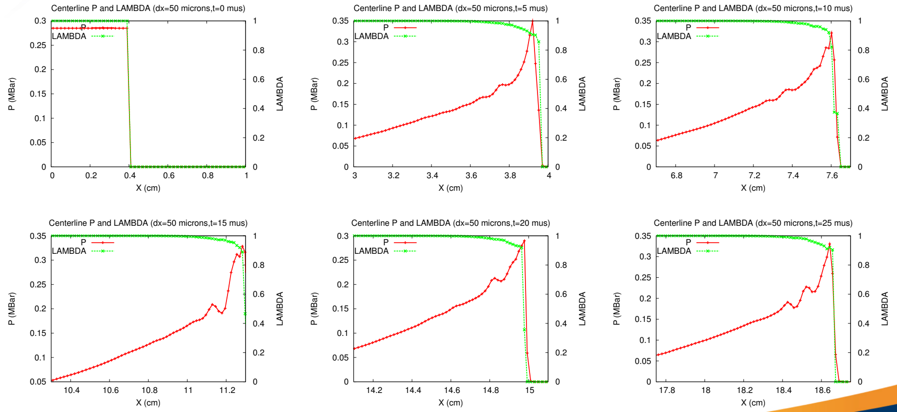
Ratestick detonation: zoom of the front

- Qualitatively the results are the same for all three calibrations
  - Simulation done for half-plane only then drawn reflected



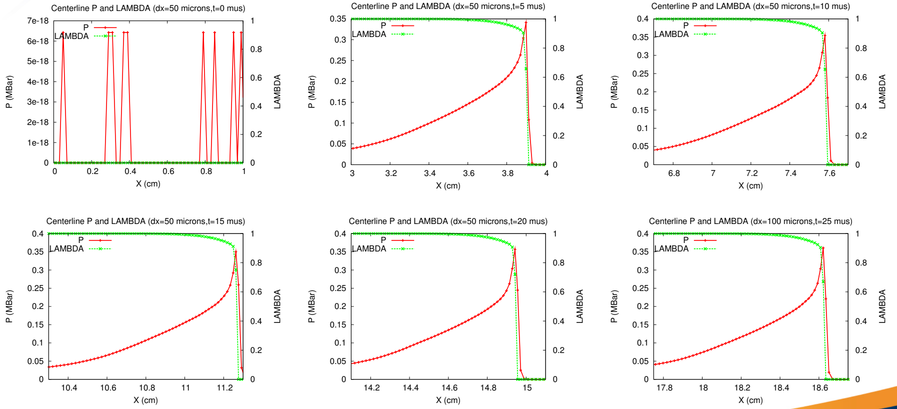
Ratestick detonation: evolution along centreline

- The burn-table employs a Dn-Kappa curve calibrated to experiment[5]
  - The *validation* of the DSD-PRZ methodology hinges on whether the FLAG hydro can remain synched with the burn-table
    - results at $dx = 100\mu m$ are non monotone



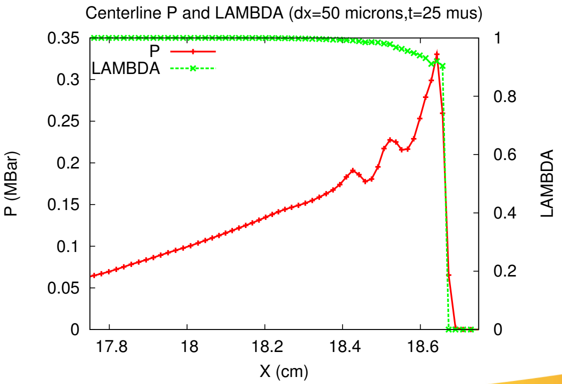
Ratestick detonation: evolution off centreline

- Pressure evolution at a radius of 4mm does not exhibit the non-monotonicty seen on the centreline
  - There may be an issue with FLAG's handling of the axis of symmetry
    - pressure plot at $t = 0$ lies outside initiation blob and can be ignored



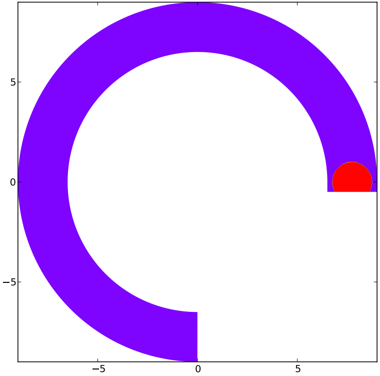
Ratestick detonation: proportioning of errors

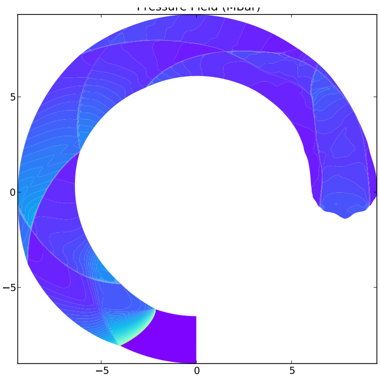
- Further investigation is needed to proportion the error
  - DSD vs. PRZ vs. FLAG vs. mesh resoluton vs. ...
  - Compared to the cylindrical case shockless burning is inhibited because Dn reaches steady state
    - but it could reappear for fine mesh simulations



Arcwave detonation

- DSD-PRZ simulations have been performed in FLAG for an arcwave† of PBX-9502[3], with the three calibrations[8, 2, 1]
  - Pressure results for calibration[1] with $dx = 100\mu m$
    - reflected shocks arise because FLAG does not have an outflow-BC

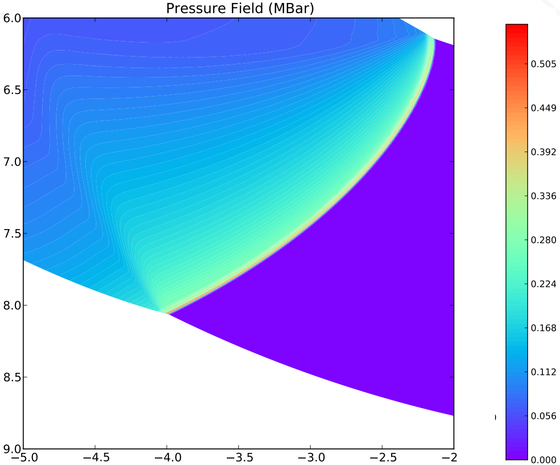




† The arcwave has 6.5mm inner radius and 9mm outer radius

Arcwave detonation: zoom of the front

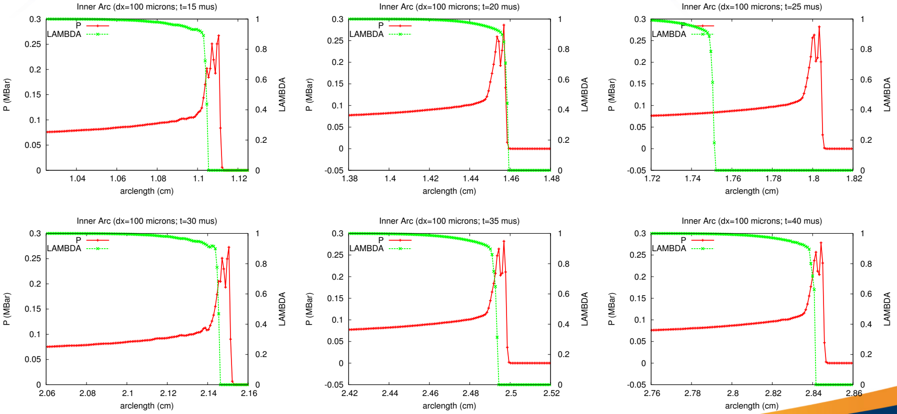
- Qualitatively the results are the same for all three calibrations
  - Observe how the front pressure increases from inner to outer radius



UNCLASSIFIED

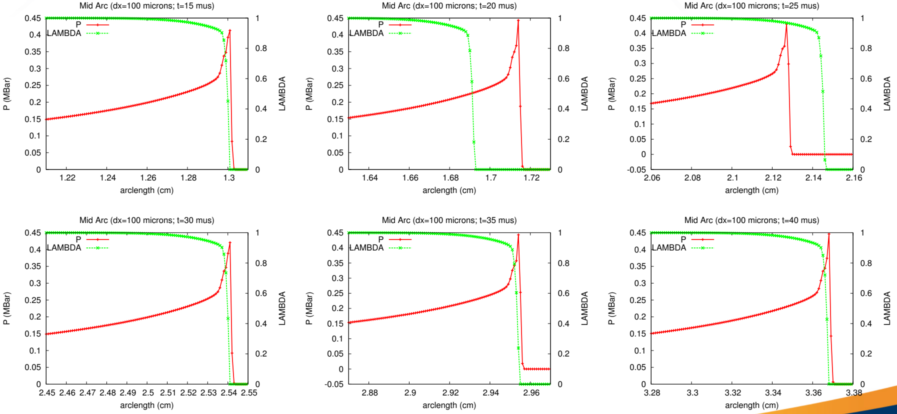
Arcwave detonation: evolution along inner arc

- The burn-table employs a Dn-Kappa curve calibrated to experiment[5]
  - The *validation* of the DSD-PRZ methodology hinges on whether the FLAG hydro can remain synched with the burn-table
    - results at $dx = 100\mu m$ are non monotone, but hint at a *flat-top*



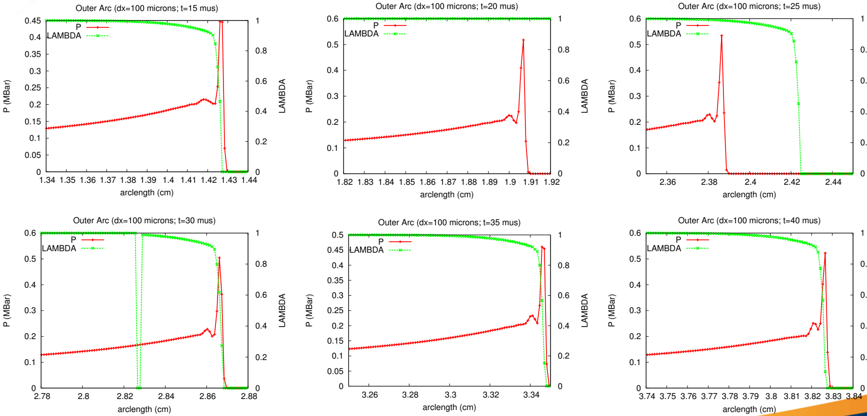
Arcwave detonation: evolution along mid arc

- The profiles for the mid-arc are monotone
  - The plots for $t = 20\mu s$ and $t = 25\mu s$ are suspicious
    - the processing of FLAG's vardumps is non-trivial and may be buggy: further investigation is required



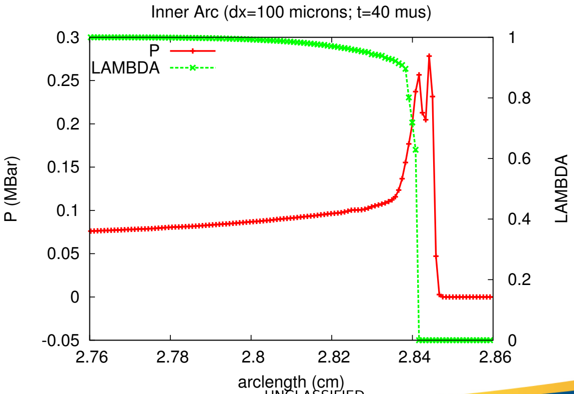
Arcwave detonation: evolution along outer arc

- The profiles for the outer-arc are non-monotone, perhaps due to FLAG's treatment of the material interface at the boundary
  - Again the plots for $t = 20\mu s$ and $t = 25\mu s$ are suspicious
    - The dropped-λ at $t = 30\mu s$ is thought to be a FLAG bug



Arcwave detonation: proportioning of errors

- Further investigation is needed to proportion the error
  - DSD vs. PRZ vs. FLAG vs. mesh resoluton vs. ...
  - Compared to the cylindrical case shockless burning is inhibited because Dn reaches steady state
    - but it could reappear for fine mesh simulations



Summary: what have we learnt?

- PRZ has been implemented correctly in FLAG
  - Although there is room for improvement in FLAG's P-T closure
  - Reliability will vary depending on the specific PRZ parameter set
    - the infinite reaction length calibration[2] falls foul of FLAG's default tolerances/thresholds
- PRZ formulation is prone to introduce shockless burning
  - More likely the higher the mesh resolution
  - Strong tendency for a cylindrical detonation
  - Inhibited for slab, ratestick, and arcwave
  - Modified/alternative PRZ formulations should be explored
- PRZ simulations in 2D should be considered *preliminary*
  - Higher resolution needed to determine limiting numerical behaviour
  - Interactions with FLAG's hydro, especially at material interfaces, is complex and requires further investigation
- PRZ, despite its mathematical shortcomings, may be an acceptable engineering-tool in FLAG for user applications

References I

[1] T.D. Aslam.
PRZ calibration for PBX 9502 – finite reaction zone (PBX9502/L2-2015b).
Technical Report LA-UR-15-27203, 2015.

[2] T.D. Aslam.
PRZ calibration for PBX 9502 – infinite reaction zone (PBX9502/L2015a).
Technical Report LA-UR-15-27335, 2015.

[3] J.B. Bdzil, T.D. Aslam, R. Henninger, and J.J. Quirk.
High-explosives performance.
Los Alamos Science, (28):96–110, 2003.

[4] W. Fickett and W.C. Davis.
Detonation: Theory and Experiment.
Dover books on physics. Dover Publications, 2000.

References II

[5] S.I. Jackson and M. Short.
Scaling of detonation velocity in cylinder and slab geometries for ideal, insensitive, and non-ideal explosives.
Journal of Fluid Mechanics, 773:224–266, 2015.

[6] A.K. Kapila, B. Bdzil, and D.S. Stewart.
On the structure and accuracy of programmed burn.
Combustion Theory and Modelling, 10(2):289–321, 2006.

[7] B.L. Wescott.
Development of a generalized pseudo-reaction zone model for non-ideal explosives and application to anfo.
Technical Report LA-UR-06-8661, 2006.

[8] B.L. Wescott, D.S. Stewart, and W.C. Davis.
Equation of state and reaction rate for condensed-phase explosives.
Journal of applied physics, 98(5):053514, 2005.